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Addition of Nitric Oxide to Hexakis(tert-butoxy)-ditungsten.
Preparation, Properties and Structural Characterization of
Tris(tert-butoxy)(nitrosyl)(pyridine)tungsten.

10 M. H. Chisholm, F. A. Cotton, M. W. Extine

R. L. Kelly

Departments of Chemistry

¹Princeton University

Princeton, New Jersey 08540

and

²Texas A & M University

College Station, Texas 77843

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Addition of Nitric Oxide to Hexakis(tert-butoxy)-ditungsten.
Preparation, Properties and Structural Characterization of
Tris(tert-butoxy)(nitrosyl)(pyridine)tungsten.

M. H. Chisholm*^{2a}, F. A. Cotton*^{2b}, M. W. Extine^{2b}
and R. L. Kelly^{2a}

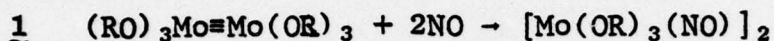
Contribution from the Departments of Chemistry, Princeton
University, Princeton, New Jersey 08540 and Texas A and M University,
College Station, Texas 77843.

Abstract

The reaction between $W_2(OBu^t)_6$ and nitric oxide (2 equiv) in hydrocarbon solvents yields an insoluble pale-yellow product of empirical formula $W(OBu^t)_3NO$ ($\nu_{NO} = 1560\text{ cm}^{-1}$). Addition of the nitrogen donor ligands NH_3 , NMe_3 and pyridine causes the above compound to dissolve with the formation of mononuclear compounds $W(OBu^t)_3(NO)(L)$. The yellow crystalline compound $W(OBu^t)_3(NO)(C_5H_5N)$ ($\nu_{NO} = 1555\text{ cm}^{-1}$) has been obtained directly by the reaction between $W_2(OBu^t)_6$ and NO (2 equiv) in pyridine as the solvent. The compound crystallizes in the space group $P2_1/n$ with $Z=4$ and unit cell dimensions $a = 9.694(2)$, $b = 15.686(3)$, $c = 14.358(2)\text{ \AA}$, $\beta = 97.40(1)^\circ$ and $V = 2165.1(7)\text{ \AA}^3$. The coordination geometry of the WO_3N_2 moiety is a slightly distorted trigonal bipyramid with the axial positions occupied by the nitrogen atoms of the nitrosyl and pyridine ligands. The tungsten atom is displaced 0.34 \AA towards the nitrosyl ligand from the equatorial plane of the three alkoxy oxygen atoms. There is a linear $W-N-O$ moiety with a short $W-N$ bond distance, $1.732(8)\text{ \AA}$, whereas the $W-N$ bond distance to the coordinated pyridine is long, $2.323(7)\text{ \AA}$.

Introduction

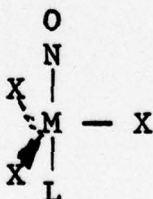
Previously we have shown that the molybdenum-to-molybdenum triple bond in the dinuclear alkoxides $\text{Mo}_2(\text{OR})_6$ ³ is cleaved in reaction 1.⁴



where $\text{R} = \text{Me}_3\text{C}$, Me_2CH and Me_3CCH_2

The structural characterization of $[\text{Mo}(\text{OPr}^i)_3\text{NO}]_2$ revealed two equivalent (inversion-related) distorted trigonal bipyramidal $\text{Mo}(\text{OR})_4\text{NO}$ units fused along a common axial-to-equatorial edge through the agency of bridging iso-propoxy groups. With a Mo-to-Mo distance of $3.335(2)\text{\AA}$ it can be safely assumed that no direct metal-to-metal bonding exists.⁵ In a formal sense reaction 1 corresponds to the replacement of the metal-to-metal triple bond by two metal-to-ligand triple bonds followed by Lewis base association,⁶

We concluded⁴ that "There would not seem to be any reason why discrete mononuclear complexes of type A, where X represents a univalent ligand, L a sigma donor, and M any atom or ion isoelectronic with $\text{Mo}(\text{III})$, should not exist as a general class."



A

We report here our preparation and characterization of the first member of this class, namely $\text{W}(\text{OBu}^t)_3(\text{NO})(\text{C}_5\text{H}_5\text{N})$, formed in the reaction between $\text{W}_2(\text{OBu}^t)_6$ and NO (2 equiv) in pyridine.

Results and Discussion

Synthesis. Addition of nitric oxide (2 equiv) to hydrocarbon solutions of $\text{W}_2(\text{OBu}^t)_6$ ⁷ leads to the formation of a fine yellow

precipitate of empirical formula $W(OBu^t)_3NO$ which shows a single sharp and very strong i.r. absorption at 1565cm^{-1} assignable to ν_{NO} . This compound is virtually insoluble in alkane and aromatic hydrocarbons which has hindered its further characterization. It is believed to be polymeric, $[W(OBu^t)_3NO]_n$, in contrast to the dimeric molybdenum analogue $[Mo(OBu^t)_3NO]_2$. $[W(OBu^t)_3NO]_n$ will dissolve in the presence of Me_3N and pyridine yielding $W(OBu^t)_3(NO)(L)$. The compound $W(OBu^t)_3(NO)(C_5H_5N)$ has also been made directly by the addition of NO (2 equiv) to a pyridine solution of $W_2(OBu^t)_6$ and is a yellow crystalline compound appreciably soluble in hydrocarbon solvents. For $W(OBu^t)_3(NO)(C_5H_5N)$ a strong sharp i.r. absorption at 1555cm^{-1} is assignable to ν_{NO} ; a sharp band of medium intensity at 1610cm^{-1} is assigned to the stretching vibration of the coordinated pyridine. The nmr spectra in toluene- d_8 of $W(OBu^t)_3(NO)(C_5H_5N)$ show the presence of only one type of tert-butoxy ligand, even at -60°C . This, together with the observation of a single nitrosyl stretching frequency, is consistent with the presence in solution of a structure akin to that found in the crystal.

Solid State Structure of $W(OBu^t)_3(NO)(C_5H_5N)$. The compound is composed of discrete mononuclear molecules in the solid state. Atomic positional and thermal parameters are given in Table I. The molecular structure is shown in Figure 1 along with the atom labelling scheme. Bond distances and angles are given in Table II. As can be seen from Figure 1, the coordination geometry is a slightly distorted trigonal bipyramid with the axial positions occupied by the nitrosyl and pyridine ligands.

The tungsten atom is displaced 0.34\AA towards the nitrosyl ligand from the equatorial plane of the three alkoxy oxygen atoms.

The nitrosyl ligand is coordinated linearly and the W-N1 bond is quite short, 1.732(8) Å, indicative of some multiple bond character whereas the tungsten to pyridine bond is considerably longer, W-N2=2.323(7) Å. The W-O distances are in the expected range.

Bonding. The trigonal set of ligands splits the tungsten 5d orbitals into three sets: a (d_{z^2}), e ($d_{x^2-y^2}$, d_{xy}) and e (d_{xz} , d_{yz}). The second e set is but little involved in metal ligand σ -bonding and thus lies lowest in energy. In $W(OBu^t)_3(NO)(py)$ tungsten achieves only a fourteen valence shell electronic configuration. Ten electrons are involved in forming the five σ bonds and the remaining four occupy the lower e orbitals which have the appropriate symmetry to interact with the empty nitrosyl π^* orbitals. The bonding is analogous to that in $[Mo(OPr^i)_3NO]_2$, where a bridging isopropoxide occupies the axial position trans to the nitrosyl ligand.

For a linear metal nitrosyl moiety, metal-to-nitrosyl π^* bonding should be reflected in (i) the metal-to-nitrogen bond distance, (ii) the nitrogen-to-oxygen bond distance and (iii) the value of the N-O stretching frequency. A lengthening of the N-O bond and a lowering of $\nu(NO)$ should correlate with an increase in metal-to-nitrosyl π^* -bonding. The shortness of the metal-to-nitrogen bond may also correlate with M-N multiple bond character but this distance will also be influenced by the nature of the metal σ -hybrid orbital used in forming the M-N bond. The latter is determined by the coordination number and geometry of the metal complex as well as by the nature of the other ligands bonded to the metal.

M-N and N-O bond distances and $\nu(NO)$ values for some compounds containing linear M-N-O moieties are given in Table 3 and are

illustrative of the above considerations. Certainly little can be inferred from the M-N distances alone. There does, however, seem to be the expected correlation between N-O bond length and $\nu(\text{NO})$. This correlation is limited, however, by the relatively small changes and large experimental errors which occur in N-O distances. One can conclude that the generally accepted view that $\nu(\text{NO})$ correlates with metal-to-nitrosyl π^* bonding finds structural support in N-O bond distances.

The trihaloruthenium complexes, which contain six coordinate metal atoms, all show very similar M-N-O parameters (see Table 3). Notably the values of $\nu(\text{NO})$ are more than 200 cm^{-1} higher, and the N-O distances are significantly shorter than those of the five coordinate molybdenum and tungsten complexes. The metals here are all in the +2 oxidation state, if we assume the formalism $\text{M}^+-(\text{NO})^+$ for the linear M-N-O moiety. Evidently the $(t_{2g})^6$ -to- $\text{NO}\pi^*$ bonding is less effective in these Ru(2+) octahedral complexes than is the $(e)^4$ -to- $\text{NO}\pi^*$ bonding in the Mo(2+) and W(2+) trigonal bipyramidal complexes, despite the presence of only 14-valence shell electrons in the latter. A plausible rationale for this observation may lie in the mixing of ligand-to-metal π -bonding (p - d) and metal-to- $\text{NO}\pi^*$ bonding. Ligand (OR or NR_2)-to-metal- π bonding in the four-coordinate $\text{Cr}(\text{NR}_2)_3\text{NO}$ and five-coordinate $\text{M}(\text{OR})_3(\text{NO})\text{L}$ molecules will raise the energy of the filled metal d_{xz} and d_{yz} atomic orbitals from the level they would otherwise have had as a result of pure M-L σ -bonding. The energy separation between filled metal d_{xz} and d_{yz} orbitals and the vacant higher energy $\text{NO}\pi^*$ orbitals will be reduced and metal-to-nitrosyl π^* bonding enhanced. It is, of course, not possible to separate completely the σ and π -donor properties of a ligand. However, the values of $\nu(\text{NO})$ do go down as the overall donor ($\sigma + \pi$) properties of the ligand increase: compare $\nu(\text{NO})=1698\text{ cm}^{-1}$ for

$\text{Cr}(\text{N}(\text{SiMe}_3)_2)_3\text{NO}$ with $\nu(\text{NO})=1640\text{ cm}^{-1}$ for $\text{Cr}(\text{NPr}^i_2)_3\text{NO}$ and $\nu(\text{NO})=1643, 1640$ and 1630 cm^{-1} for the compounds $[\text{Mo}(\text{OR})_3\text{NO}]_2$ where $\text{R} = \text{CH}_2\text{CMe}_3, \text{CHMe}_2$ and CMe_3 , respectively.

Experimental Section

General procedures have been described;¹ note the use of dry and oxygen free atmospheres and solvents.

$\text{W}_2(\text{OBu}^t)_6$ was prepared from the reaction between $\text{W}_2(\text{NMe}_2)_6$ and Bu^tOH (> 6 equiv) in benzene and was recrystallized from hexane solutions.⁷

$[\text{W}(\text{OBu}^t)_3\text{NO}]_n$: $\text{W}_2(\text{OBu}^t)_6$ (0.63g, 0.78 mmol) was dissolved in hexane (10 mL) to give a red solution. Nitric oxide (1.56 mmol) was added with the use of a calibrated manifold to the above solution frozen at liquid nitrogen temperature which yielded upon warming to room temperature a green solution and a pale yellow precipitate. After 5h the pale yellow precipitate was collected by filtration, washed with hexane, and dried in vacuo (10^{-4} cm Hg, 25°C). Yield 0.56g (83% based on tungsten). Analysis found (calcd) for $\text{W}(\text{OBu}^t)_3\text{NO}$: C, 33.06 (33.27); H, 6.20 (6.28); N, 3.40 (3.23).

I.r. data obtained from a nujol mull between CsI plates (2000-300 cm^{-1} range): 1565 vs, 1310 w, 1245 m, 1165 s (broad), 1090 s, 1030 w, 948 vs (broad), 928 vs, 912 s, 796 m (sharp), 784 m (sharp), 724 m (broad), 627 s (sharp), 595 m, 572 m, 485 w, 394 w, 381 w, 340 w.

$\text{W}(\text{OBu}^t)_3(\text{NO})(\text{C}_5\text{H}_5\text{N})$: $\text{W}_2(\text{OBu}^t)_6$ (0.1844g, 0.23 mmol) was dissolved in pyridine (7 ml) to form a deep red solution. This was frozen at liquid nitrogen temperature and nitric oxide (0.46 mmol) was added using a calibrated vacuum manifold. The reaction mixture was allowed to warm to room temperature and left to stand for 12h. The pyridine was stripped and the residue extracted with

toluene (ca. 5 mL). The pale yellow solution was filtered to remove a small amount of a black insoluble material. The filtrate was collected and cooled to -10°C yielding pale yellow crystals (ca. 80 mg). Analysis found (calcd) for $\text{W}(\text{OBu}^t)_3(\text{NO})(\text{C}_5\text{H}_5\text{N})$: C, 39.65 (39.86); H, 6.25 (6.30); N, 5.40 (5.47). I.r. data obtained from a nujol mull using CsI plate in the range $2000\text{--}300\text{ cm}^{-1}$: 1610 m (sharp), 1555 vs, 1305 w, 1240 m, 1222 m (sharp), 1170 m (broad), 1156 m (sharp), 1076 m (sharp), 1043 m (sharp), 1027 w, 1018 w, 1000 w, 965 m, 948 m, 937 vs (broad), 910 m, 900 w, 783 m, 762 m (sharp), 722 m (broad), 694 m (sharp), 621 s, 576 m, 485 w, 436 w, 380 w.

^{13}C nmr data obtained in toluene- d_8 at -50°C : $\delta(\text{OC}) = 80.8$, $\delta(\text{CH}_3) = 32.9$. (δ in ppm rel. TMS).

X-Ray Crystallography.⁸ A yellow crystal of $\text{W}(\text{OBu}^t)_3(\text{NO})(\text{C}_5\text{H}_5\text{N})$ measuring $0.23 \times 0.28 \times 0.58\text{ mm}$ was mounted, embedded in epoxy cement and sealed in a thin walled glass capillary, with its longest dimension nearly coincident with the ϕ axis. Omega scans of several intense low-angle reflections had peak widths at half height of ca. 0.2° . Cell constants and axial photographs indicated that the crystal belonged to the monoclinic system with $a = 9.694(2)$, $b = 15.686(3)$, $c = 14.358(2)\text{\AA}$, $\beta = 97.40(1)^{\circ}$, and $V = 2165.1(7)\text{\AA}^3$. The observed volume was consistent with that expected for $Z = 4$. Systematic absences observed during data collection, on $0k0$ ($k = 2n+1$) and $h0l$ ($h+l = 2n+1$), uniquely determined the space group to be $\text{P}2_1/\text{n}$ (a non-standard setting of $\text{P}2_1/\text{c}$, No. 14).

The data were collected at $23 \pm 2^{\circ}\text{C}$ with a Syntex $\text{P}\bar{\text{I}}$ autodiffractometer equipped with a graphite crystal monochromator and using $\text{MoK}\alpha$ ($\lambda = 0.710730\text{\AA}$) radiation. Variable scan rates from 4.8 to $24.0^{\circ}/\text{min}$ were used for symmetric $\theta/2\theta$ scans ranging from 1.0° below to 1.0° above the calculated $\text{MoK}\alpha_1, \text{K}\alpha_2$ doublet. The

ratio of background to scan time was 0.5. A total of 2936 unique reflections having $0^\circ < 2\theta_{\text{MoK}\alpha} < 45^\circ$ were collected. The intensities of three standard reflections were monitored frequently throughout data collection and showed an approximately linear decrease of 12% over the period of data collection. The data were reduced to a set of relative $|F_o|^2$ values and then corrected for crystal decay. An empirical absorption correction based upon a series of psi scans was applied to the data ($\mu = 56.7 \text{ cm}^{-1}$); relative transmission factors ranged from 0.844 to 1.000 with an average of 0.949. The 2103 observations having $|F| > 3\sigma(|F|)$ were retained as observed and used in subsequent structure solution and refinement.

The positions of the 24 unique non-hydrogen atoms were determined by standard heavy atom methods. The structure was refined to convergence using anisotropic thermal parameters for all 24 atoms. The final discrepancy indices were

$$R_1 = \sum ||F_o| - |F_c|| / \sum |F_o| = 0.032$$

$$R_2 = [\sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2]^{1/2} = 0.047$$

The estimated standard deviation of an observation of unit weight was 1.102. The top peaks in a final difference Fourier map were due to methyl group hydrogen atoms.

A table of observed and calculated structure factors (9 pages) is available as supplementary material. See any current masthead page for ordering information.

Acknowledgements

We thank the Office of Naval Research for support of this work at Princeton University and the National Science Foundation for support at Texas A & M University.

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5. A good comparison can be made between two structurally related compounds $\text{Mo}_2(\text{OPr}^i)_6(\text{NO})_2$ and $\text{Mo}_2(\text{OPr}^i)_8$. The latter has a Mo-to-Mo distance of $2.525(2)\text{\AA}$ indicative of a metal-to-metal double bond. M. H. Chisholm, F. A. Cotton, M. W. Extine and W. W. Reichert, Inorg. Chem. submitted for publication.
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8. All crystallographic computations were carried out using the Enraf Nonius Structure Determination Package and a PDP11/45 computer owned by Molecular Structure Corp., College Station, Texas.

TABLE I. POSITIONAL AND THERMAL PARAMETERS AND THEIR ESTIMATED STANDARD DEVIATIONS.

ATOM	X	Y	Z	$\sigma(1.1)$	$\sigma(2.2)$	$\sigma(3.3)$	$\sigma(1.2)$	$\sigma(1.3)$	$\sigma(2.3)$
W	0.05941(4)	0.23082(3)	0.08295(2)	2.90(1)	3.59(2)	2.80(1)	-0.09(1)	0.56(1)	0.45(1)
O1	-0.0626(6)	0.1482(4)	0.0250(4)	3.9(3)	4.4(3)	3.3(3)	-0.4(3)	-0.5(2)	0.4(3)
O2	0.2467(6)	0.1974(4)	0.1196(4)	3.2(3)	4.8(3)	3.5(3)	-0.0(2)	0.9(2)	0.7(2)
O3	-0.0194(6)	0.3097(4)	0.1602(4)	4.1(3)	3.6(3)	3.8(3)	0.0(3)	1.3(2)	0.7(2)
O4	0.0918(8)	0.3428(5)	-0.0806(5)	7.0(4)	5.7(4)	4.5(3)	0.6(3)	2.1(3)	2.6(3)
N1	0.0779(8)	0.2964(5)	-0.0117(5)	4.0(3)	4.5(4)	4.1(4)	0.4(3)	1.0(3)	1.1(3)
N2	0.0280(7)	0.1486(5)	0.2131(5)	2.8(3)	4.1(3)	3.1(3)	-0.3(3)	0.7(3)	0.1(3)
C1	-0.1302(11)	0.1312(7)	-0.0713(7)	5.4(5)	4.9(5)	3.0(4)	-0.1(4)	-0.8(4)	-0.6(4)
C2	-0.0145(13)	0.1150(9)	-0.1326(8)	8.0(7)	8.8(7)	3.3(5)	1.5(6)	-0.3(5)	-1.7(5)
C3	-0.2176(13)	0.2086(7)	-0.1062(9)	6.3(6)	4.9(6)	6.7(6)	0.8(5)	-0.7(5)	1.2(5)
C4	-0.2203(13)	0.0515(8)	-0.0594(9)	7.1(7)	6.0(6)	6.5(6)	-2.6(5)	-2.1(6)	0.2(5)
C5	0.3771(10)	0.2141(7)	0.0837(8)	3.2(4)	6.5(7)	5.4(5)	-0.3(4)	1.4(4)	0.3(5)
C6	0.4030(12)	0.3098(9)	0.0875(9)	6.2(6)	6.8(6)	8.5(7)	-2.7(5)	2.5(5)	-1.0(6)
C7	0.3682(11)	0.1819(9)	-0.0177(7)	5.2(5)	9.0(7)	4.1(5)	-0.2(6)	1.9(4)	-1.5(5)
C8	0.4869(11)	0.1626(10)	0.1500(9)	3.1(5)	12(1)	6.0(6)	1.0(6)	0.1(5)	1.0(7)
C9	-0.0600(10)	0.3984(6)	0.1535(7)	4.2(4)	3.4(4)	4.4(4)	-0.0(4)	1.2(4)	0.6(4)
C10	0.0691(11)	0.4526(7)	0.1492(8)	4.9(5)	4.2(5)	6.6(6)	-0.6(4)	0.4(5)	0.3(5)
C11	-0.1205(13)	0.4164(7)	0.2459(8)	10.7(7)	5.1(6)	4.9(5)	2.4(5)	3.7(5)	-0.1(4)
C12	-0.1686(11)	0.4125(7)	0.0670(8)	4.7(5)	5.9(6)	4.6(5)	1.2(4)	-0.4(4)	1.3(4)
C13	0.1261(9)	0.1046(6)	0.2641(6)	4.0(4)	3.9(4)	3.2(4)	1.1(4)	0.4(3)	0.3(4)
C14	0.1021(10)	0.0589(7)	0.3437(7)	3.9(5)	6.0(6)	4.3(5)	0.4(4)	0.2(4)	1.2(4)
C15	-0.0289(12)	0.0605(7)	0.3711(7)	6.5(6)	6.4(6)	3.4(4)	0.4(5)	1.0(4)	1.6(4)
C16	-0.1333(11)	0.1066(7)	0.3181(7)	5.6(5)	4.6(5)	4.9(5)	-0.4(4)	2.5(4)	1.0(4)
C17	-0.1003(10)	0.1497(7)	0.2390(7)	3.6(4)	4.5(5)	5.6(5)	-0.3(4)	0.9(4)	1.8(4)

The form of the anisotropic thermal parameter is:

$$\exp[-1/4(B_{11}h^2a^2 + B_{22}k^2b^2 + B_{33}l^2c^2 + 2B_{12}hka^*b^* + 2B_{13}hla^*c^* + 2B_{23}klb^*c^*)]$$

Table II. Bond Distances (Å) and Angles (Deg) in $W(OBu^t)_3(NO)(C_5H_5N)^a$

ATOMS -----			DISTANCE -----	ATOMS -----			DISTANCE -----
W	O1		1.876(6)	C1	C3		1.527(15)
W	O2		1.898(6)	C1	C4		1.547(15)
W	O3		1.887(6)	C5	C6		1.52(2)
W	N1		1.732(8)	C5	C7		1.533(15)
W	N2		2.323(7)	C5	C8		1.560(15)
O1	C1		1.476(11)	C9	C10		1.520(14)
O2	C5		1.449(11)	C9	C11		1.544(14)
O3	C9		1.446(11)	C9	C12		1.538(14)
O4	N1		1.250(10)	C13	C14		1.394(13)
N2	C13		1.318(11)	C14	C15		1.377(14)
N2	C17		1.343(11)	C15	C16		1.389(14)
C1	C2		1.53(2)	C16	C17		1.393(13)

ATOMS -----				ATOMS -----				ANGLE -----
O1	W	O2	117.3(3)	C2	C1	C3		111.(1)
O1	W	O3	115.7(3)	C2	C1	C4		113.(1)
O1	W	N1	100.7(3)	C3	C1	C4		112.(1)
O1	W	N2	80.4(3)	O2	C5	C6		108.3(9)
O2	W	O3	117.6(3)	O2	C5	C7		109.5(8)
O2	W	N1	100.9(3)	O2	C5	C8		104.3(8)
O2	W	N2	81.0(2)	C6	C5	C7		110.(1)
O3	W	N1	99.4(3)	C6	C5	C8		113.(1)
O3	W	N2	77.7(3)	C7	C5	C8		111.(1)
N1	W	N2	177.0(3)	O3	C9	C10		108.8(8)
W	O1	C1	135.9(6)	O3	C9	C11		104.4(8)
W	O2	C5	134.3(6)	O3	C9	C12		110.1(8)
W	O3	C9	136.0(5)	C10	C9	C11		110.(1)
W	N1	O4	179.2(8)	C10	C9	C12		111.6(9)
W	N2	C13	125.3(6)	C11	C9	C12		111.8(9)
W	N2	C17	116.0(6)	N2	C13	C14		122.7(9)
C13	N2	C17	118.7(8)	C13	C14	C15		118.8(9)
O1	C1	C2	107.4(8)	C14	C15	C16		119.1(9)
O1	C1	C3	108.9(8)	C15	C16	C17		118.(1)
O1	C1	C4	103.3(8)	N2	C17	C16		122.6(9)

^aNumbers in parentheses are estimated standard deviations in the least significant digits.

Table III

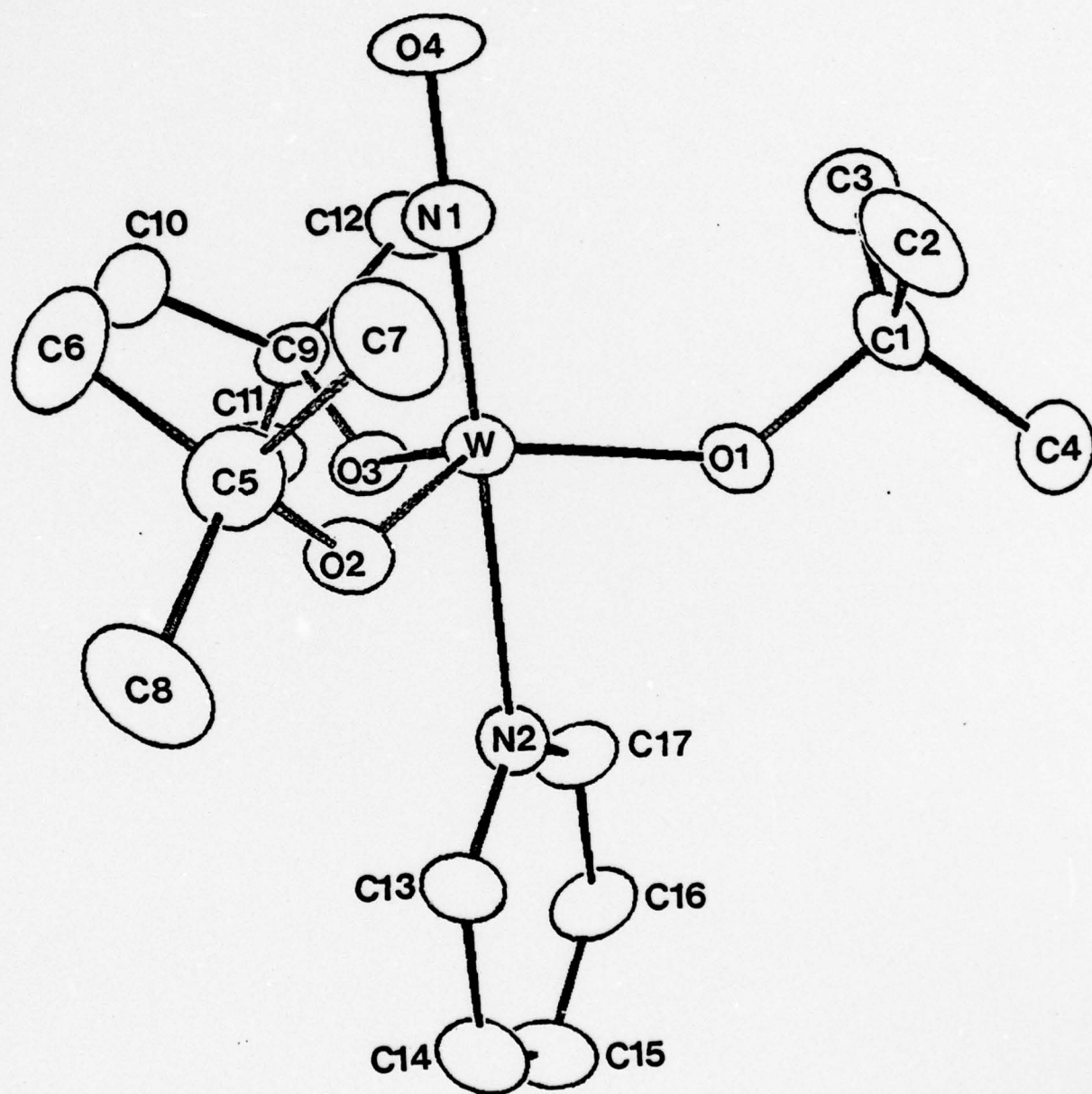
Compound	M-N Δ	N-O Δ	M-N-O angle ^o	$\nu(\text{NO})\text{cm}^{-1}$	ref.
$\text{W}(\text{OBU}^t)_3(\text{NO})(\text{pyridine})$	1.732(8)	1.25(1)	179.2(8)	1555	a
$[\text{Mo}(\text{OPr}^f)_3\text{NO}]_2$	1.754(7)	1.19(1)	178(1)	1640	b
$\text{Cr}(\text{NSi}_2\text{Me}_6)_3\text{NO}$	1.738(20)	1.191(28)	180 ⁱ	1698 ^j	c
$\text{Ru}(\eta^3\text{-allyl})(\text{NO})(\text{PPh}_3)_2$	1.751(6)	1.188(8)	173.8(6)	1640	d
$\text{RuCl}_3(\text{NO})(\text{PPh}_3)_2$	1.737(7)	1.142(8)	180 ⁱ	1876	e
$\text{RuCl}_3(\text{NO})(\text{PPh}_2\text{Me})_2$	1.744(6)	1.132(6)	176.4(6)	1860 ^k	f
$[\text{RuBr}_3(\text{NO})(\text{Et}_2\text{SO})]_2$	1.71(1)	1.16(1)	178(1)	1874	g
$[\text{Mo}(\text{CN})_5\text{NO}]^{4-}$	1.95(3)	1.23(4)	175(3)	1455 ^l	h

^a this work; ^b ref.4; ^c D. C. Bradley, M. B. Hursthouse, C. W. Newing and A. J. Welch, J.C.S. Chem. Commun, 567 (1972); ^d M. W. Schoonover and R. Eisenberg, J. Am. Chem. Soc. 99, 8371 (1977); ^e B. L. Haymore and J. A. Ibers, Inorg. Chem. 14, 3060 (1975); ^f A. J. Schultz,

R. L. Henry and R. Eisenberg, Inorg. Chem. 13, 732 (1974); ^g J. E. Fergusson, C. T. Page and W. T. Robinson, Inorg. Chem., 15, 2270 (1976); ^h D. H. Svedung and N.-G. Vannerberg, Acta. Chem. Scand. 22, 1551 (1968); ⁱ crystallographically imposed linearity; ^j C. W. Newing, Ph.D. Thesis London University 1971; ^k J. Chatt and B. L. Shaw, J. Chem. Soc., A, 1811 (1966).

^l R.F. Riley and L. Ho, J. Inorg. Nucl. Chem. 24, 1121 (1962).

Figure 1. An ORTEP view of the $\text{W}(\text{OBu}^t)_3(\text{NO})(\text{C}_5\text{H}_5\text{N})$ molecule using 40% probability ellipsoids and showing the atom numbering scheme.



H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
1	1	1	437	456	1	1	1	1461	1508	1	1	1	163	194	1	1	1	1065	1022	1	1	1	827	816
1	1	1	251	220	1	1	1	1101	1119	1	1	1	1065	1022	1	1	1	499	556	1	1	1	255	268
1	1	1	663	688	1	1	1	857	879	1	1	1	335	303	1	1	1	335	303	1	1	1	206	183
1	1	1	233	249	1	1	1	236	256	1	1	1	468	495	1	1	1	468	495	1	1	1	1137	1138
1	1	1	832	852	1	1	1	513	531	1	1	1	627	631	1	1	1	627	631	1	1	1	531	525
1	1	1	692	695	1	1	1	249	248	1	1	1	571	584	1	1	1	571	584	1	1	1	824	818
1	1	1	508	521	1	1	1	280	314	1	1	1	281	309	1	1	1	281	309	1	1	1	586	579
1	1	1	535	454	1	1	1	347	414	1	1	1	405	407	1	1	1	405	407	1	1	1	623	614
1	1	1	444	454	1	1	1	568	584	1	1	1	371	336	1	1	1	371	336	1	1	1	680	725
1	1	1	1371	1370	1	1	1	1070	1008	1	1	1	498	477	1	1	1	498	477	1	1	1	1022	1011
1	1	1	397	368	1	1	1	457	457	1	1	1	330	335	1	1	1	330	335	1	1	1	181	164
1	1	1	117	1031	1	1	1	939	927	1	1	1	1120	1150	1	1	1	1120	1150	1	1	1	656	665
1	1	1	1047	1415	1	1	1	1519	1519	1	1	1	850	840	1	1	1	850	840	1	1	1	534	535
1	1	1	1219	1121	1	1	1	5822	5822	1	1	1	407	348	1	1	1	407	348	1	1	1	2753	2713
1	1	1	2037	1984	1	1	1	1344	1344	1	1	1	379	394	1	1	1	379	394	1	1	1	619	606
1	1	1	539	542	1	1	1	555	655	1	1	1	1210	1289	1	1	1	1210	1289	1	1	1	347	356
1	1	1	1793	1699	1	1	1	818	854	1	1	1	210	185	1	1	1	210	185	1	1	1	185	150
1	1	1	1049	1095	1	1	1	1127	1145	1	1	1	584	606	1	1	1	584	606	1	1	1	347	356
1	1	1	648	599	1	1	1	469	469	1	1	1	1000	1033	1	1	1	1000	1033	1	1	1	569	566
1	1	1	1644	1678	1	1	1	823	823	1	1	1	362	356	1	1	1	362	356	1	1	1	514	502
1	1	1	788	800	1	1	1	1573	1573	1	1	1	949	925	1	1	1	949	925	1	1	1	270	262
1	1	1	728	723	1	1	1	334	326	1	1	1	1152	1170	1	1	1	1152	1170	1	1	1	647	640
1	1	1	469	443	1	1	1	940	984	1	1	1	852	832	1	1	1	852	832	1	1	1	577	579
1	1	1	1017	1025	1	1	1	2274	2274	1	1	1	155	192	1	1	1	155	192	1	1	1	529	527
1	1	1	442	425	1	1	1	227	257	1	1	1	1046	1104	1	1	1	1046	1104	1	1	1	529	527
1	1	1	398	391	1	1	1	227	257	1	1	1	715	753	1	1	1	715	753	1	1	1	529	527
1	1	1	511	499	1	1	1	229	308	1	1	1	475	491	1	1	1	475	491	1	1	1	529	527
1	1	1	861	891	1	1	1	419	426	1	1	1	833	866	1	1	1	833	866	1	1	1	529	527
1	1	1	1167	1188	1	1	1	437	441	1	1	1	833	866	1	1	1	833	866	1	1	1	529	527
1	1	1	925	900	1	1	1	229	199	1	1	1	698	688	1	1	1	698	688	1	1	1	529	527
1	1	1	1468	1465	1	1	1	648	646	1	1	1	243	243	1	1	1	243	243	1	1	1	529	527
1	1	1	831	792	1	1	1	785	802	1	1	1	406	406	1	1	1	406	406	1	1	1	529	527
1	1	1	2148	2137	1	1	1	905	916	1	1	1	770	794	1	1	1	770	794	1	1	1	529	527
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1	1	1	730	612	1	1	1	1202	1191	1	1	1	612	625	1	1	1	612	625	1	1	1	529	527
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1	1	1	2022	2020	1	1	1	1326	1333	1	1	1	185	181	1	1	1	185	181	1	1	1	529	527
1	1	1	880	870	1	1	1	1326	1333	1	1	1	185	181	1	1	1	185	181	1	1	1	529	527
1	1	1	962	931	1	1	1	1326	1333	1	1	1	185	181	1	1	1	185	181	1	1	1	529	527
1	1	1	1123	1131	1	1	1	1326	1333	1	1	1	185	181	1	1	1	185	181	1	1	1	529	527
1	1	1	1024	1039	1	1	1	1326	1333	1	1	1	185	181	1	1	1	185	181	1	1	1	529	527
1	1	1	349	347	1	1	1	1012	1039	1	1	1	1012	1039	1	1	1	1012	1039	1	1	1	529	527

H	K	L	F0BS	FCALC	H	K	L	F0BS	FCALC	H	K	L	F0BS	FCALC	F0BS	FCALC
2	2	2	454	394	2	2	2	1115	1117	2	2	2	598	570	468	423
2	2	2	1148	1122	2	2	2	883	848	2	2	2	752	736	1101	1140
2	2	2	310	284	2	2	2	331	305	2	2	2	406	392	1507	1524
2	2	2	821	794	2	2	2	321	303	2	2	2	222	208	289	303
2	2	2	1533	1511	2	2	2	7495	720	2	2	2	585	573	815	837
2	2	2	416	391	2	2	2	4820	514	2	2	2	585	573	1045	1100
2	2	2	531	501	2	2	2	780	465	2	2	2	305	275	358	364
2	2	2	1585	1551	2	2	2	1022	1036	2	2	2	746	727	602	604
2	2	2	587	516	2	2	2	205	183	2	2	2	579	577	802	804
2	2	2	1935	1874	2	2	2	1837	1843	2	2	2	845	847	703	706
2	2	2	622	628	2	2	2	1094	1056	2	2	2	555	559	325	328
2	2	2	1304	1196	2	2	2	764	659	2	2	2	316	296	701	700
2	2	2	475	424	2	2	2	1084	995	2	2	2	1291	1276	575	563
2	2	2	794	619	2	2	2	1825	1796	2	2	2	328	322	465	455
2	2	2	683	2508	2	2	2	2314	2328	2	2	2	1561	1522	1192	1173
2	2	2	212	169	2	2	2	837	811	2	2	2	384	377	737	733
2	2	2	472	488	2	2	2	1256	1276	2	2	2	1597	1574	980	983
2	2	2	348	299	2	2	2	434	445	2	2	2	684	720	343	311
2	2	2	968	964	2	2	2	173	215	2	2	2	825	758	998	1040
2	2	2	1413	1404	2	2	2	1491	1487	2	2	2	704	729	205	206
2	2	2	226	219	2	2	2	378	392	2	2	2	766	743	621	694
2	2	2	433	411	2	2	2	437	426	2	2	2	533	543	233	203
2	2	2	305	268	2	2	2	586	591	2	2	2	110	113	1070	1068
2	2	2	504	590	2	2	2	281	308	2	2	2	455	472	502	472
2	2	2	813	823	2	2	2	622	642	2	2	2	454	514	561	555
2	2	2	865	869	2	2	2	394	385	2	2	2	505	519	1224	1288
2	2	2	201	239	2	2	2	394	354	2	2	2	454	519	855	830
2	2	2	221	219	2	2	2	1455	1430	2	2	2	256	249	249	225
2	2	2	1784	1803	2	2	2	1247	1229	2	2	2	663	674	709	719
2	2	2	155	1555	2	2	2	1268	1229	2	2	2	209	206	411	401
2	2	2	1166	1066	2	2	2	1234	1131	2	2	2	634	620	309	305
2	2	2	829	734	2	2	2	684	582	2	2	2	470	451	787	766
2	2	2	947	891	2	2	2	972	914	2	2	2	34	328	581	570
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2	2	2	593	567	2	2	2	933	885	2	2	2	1518	1356	817	821
2	2	2	139	116	2	2	2	530	488	2	2	2	170	187	1266	1258
2	2	2	1450	1464	2	2	2	483	394	2	2	2	1514	1492	1049	1016
2	2	2	1258	1301	2	2	2	1662	1596	2	2	2	767	795	1163	1151
2	2	2	281	308	2	2	2	632	619	2	2	2	1038	992	820	832
2	2	2	403	401	2	2	2	204	172	2	2	2	1	1	1	1

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10*FOBS & 10*FCALC FOR W(O-T-BU)3(CSH5N) (NO) [COTTON, CHISHOLM ET AL 1978]										PAGE 4									
H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
2	2	2	662	637	3	3	3	400	234	3	3	3	480	477	3	3	3	312	283
10	10	10	510	340	15	15	15	758	173	15	15	15	889	860	15	15	15	562	581
11	11	11	619	191	22	22	22	274	1569	22	22	22	209	154	22	22	22	602	521
11	11	11	653	647	22	22	22	468	183	22	22	22	780	809	22	22	22	672	653
11	11	11	855	849	22	22	22	648	1501	22	22	22	372	348	22	22	22	557	556
11	11	11	261	270	22	22	22	416	770	22	22	22	121	1228	22	22	22	830	816
11	11	11	766	561	22	22	22	445	401	22	22	22	1211	1211	22	22	22	980	913
11	11	11	1023	1096	22	22	22	564	551	22	22	22	517	495	22	22	22	983	922
11	11	11	273	258	22	22	22	742	354	22	22	22	1815	951	22	22	22	1021	1055
11	11	11	549	515	22	22	22	234	1934	22	22	22	1854	1708	22	22	22	1297	1252
11	11	11	801	819	22	22	22	1607	1522	22	22	22	1642	363	22	22	22	337	342
11	11	11	169	188	22	22	22	1350	336	22	22	22	361	262	22	22	22	1137	1126
11	11	11	308	291	22	22	22	501	103	22	22	22	427	485	22	22	22	1211	1189
11	11	11	728	891	22	22	22	1455	1654	22	22	22	1435	1480	22	22	22	333	300
11	11	11	238	310	22	22	22	1791	201	22	22	22	1634	1533	22	22	22	1010	1033
11	11	11	568	313	22	22	22	300	1659	22	22	22	762	607	22	22	22	1349	1432
11	11	11	968	610	22	22	22	1964	58	22	22	22	856	767	22	22	22	1039	1126
11	11	11	232	595	22	22	22	993	543	22	22	22	792	846	22	22	22	907	906
11	11	11	822	227	22	22	22	292	1280	22	22	22	321	346	22	22	22	551	525
11	11	11	102	835	22	22	22	1444	219	22	22	22	399	365	22	22	22	535	494
11	11	11	825	763	22	22	22	1053	2369	22	22	22	408	840	22	22	22	518	534
11	11	11	1102	1125	22	22	22	643	1268	22	22	22	430	417	22	22	22	615	607
11	11	11	825	916	22	22	22	1466	1268	22	22	22	408	417	22	22	22	456	456
11	11	11	525	210	22	22	22	1821	451	22	22	22	430	409	22	22	22	331	330
11	11	11	257	242	22	22	22	1308	671	22	22	22	542	547	22	22	22	858	859
11	11	11	257	377	22	22	22	247	834	22	22	22	199	206	22	22	22	470	447
11	11	11	257	541	22	22	22	2129	1268	22	22	22	1277	1286	22	22	22	1023	1026
11	11	11	257	236	22	22	22	211	451	22	22	22	1893	1877	22	22	22	677	677
11	11	11	257	236	22	22	22	979	671	22	22	22	665	709	22	22	22	556	581
11	11	11	257	567	22	22	22	411	1268	22	22	22	825	824	22	22	22	1133	1091
11	11	11	257	435	22	22	22	1524	655	22	22	22	1183	1144	22	22	22	551	515
11	11	11	257	681	22	22	22	2712	672	22	22	22	1820	1835	22	22	22	622	673
11	11	11	257	435	22	22	22	1388	1123	22	22	22	295	301	22	22	22	351	313
11	11	11	257	241	22	22	22	85	1073	22	22	22	889	883	22	22	22	443	410
11	11	11	257	205	22	22	22	1150	2330	22	22	22	929	906	22	22	22	1164	1177
11	11	11	257	486	22	22	22	1259	2330	22	22	22	671	619	22	22	22	517	512
11	11	11	257	142	22	22	22	307	2330	22	22	22	1131	1161	22	22	22	300	314
11	11	11	257	120	22	22	22	307	2330	22	22	22	275	304	22	22	22	268	283
11	11	11	257	627	22	22	22	307	2330	22	22	22	328	355	22	22	22	568	593
11	11	11	257	925	22	22	22	1487	1494	22	22	22	328	355	22	22	22	568	593
11	11	11	257	590	22	22	22	507	2330	22	22	22	328	355	22	22	22	568	593
11	11	11	257	204	22	22	22	233	2330	22	22	22	328	355	22	22	22	568	593

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4	4	4	572	553	4	4	4	1182	1161	4	4	4	699	657	4	4	4	456	450	4	4	4	336	338
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10*FOBS & 10*FCALC FOR W(O-T-BU)3(CSHSN) (NO) [COTTON, CHISHOLM ET AL 1978]

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H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
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6	6	11	238	216	6	8	3	508	549	6	8	3	508	549	6	8	3	508	549	6	8	3	508	549	6	8	3	508	549
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6	6	11	312	339	6	8	7	486	523	6	8	7	486	523	6	8	7	486	523	6	8	7	486	523	6	8	7	486	523
6	6	11	804	820	6	8	8	357	348	6	8	8	357	348	6	8	8	357	348	6	8	8	357	348	6	8	8	357	348
6	6	11	672	672	6	8	9	309	286	6	8	9	309	286	6	8	9	309	286	6	8	9	309	286	6	8	9	309	286
6	6	11	1050	1022	6	8	10	444	416	6	8	10	444	416	6	8	10	444	416	6	8	10	444	416	6	8	10	444	416
6	6	11	588	618	6	8	11	452	456	6	8	11	452	456	6	8	11	452	456	6	8	11	452	456	6	8	11	452	456
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H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
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6	5	7	216	237	6	5	7	649	824	7	7	7	1278	1315	7	7	7	785	766	7	7	7	309	348
6	5	7	641	661	6	5	7	231	229	7	7	7	419	425	7	7	7	623	661	7	7	7	416	365
6	5	7	828	630	6	5	7	734	338	7	7	7	764	739	7	7	7	808	801	7	7	7	929	930
6	5	7	139	168	6	5	7	834	468	7	7	7	1341	1241	7	7	7	918	961	7	7	7	445	442
6	5	7	468	462	6	5	7	539	371	7	7	7	306	306	7	7	7	623	661	7	7	7	361	368
6	5	7	635	606	6	5	7	741	546	7	7	7	483	431	7	7	7	775	793	7	7	7	415	442
6	5	7	404	476	6	5	7	625	610	7	7	7	221	207	7	7	7	630	604	7	7	7	272	269
6	5	7	381	358	6	5	7	240	601	7	7	7	481	483	7	7	7	728	714	7	7	7	287	270
6	5	7	753	725	6	5	7	416	601	7	7	7	289	221	7	7	7	407	372	7	7	7	256	269
6	5	7	511	503	6	5	7	297	225	7	7	7	383	307	7	7	7	345	361	7	7	7	215	214
6	5	7	554	566	6	5	7	651	464	7	7	7	1010	974	7	7	7	517	529	7	7	7	224	189
6	5	7	397	598	6	5	7	459	694	7	7	7	240	1005	7	7	7	355	309	7	7	7	256	414
6	5	7	244	598	6	5	7	513	643	7	7	7	975	276	7	7	7	404	384	7	7	7	295	334
6	5	7	519	498	6	5	7	606	643	7	7	7	488	1601	7	7	7	458	384	7	7	7	406	590
6	5	7	135	135	6	5	7	881	882	7	7	7	385	991	7	7	7	583	458	7	7	7	598	601
6	5	7	230	151	6	5	7	614	882	7	7	7	791	481	7	7	7	427	452	7	7	7	468	438
6	5	7	235	135	6	5	7	1355	1009	7	7	7	209	390	7	7	7	583	503	7	7	7	515	539
6	5	7	579	457	6	5	7	1059	1516	7	7	7	935	168	7	7	7	201	241	7	7	7	638	629
6	5	7	876	443	6	5	7	3393	3435	7	7	7	144	935	7	7	7	617	262	7	7	7	372	344
6	5	7	393	849	6	5	7	1162	8435	7	7	7	244	1179	7	7	7	563	543	7	7	7	476	499
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